Modeling Phytoremediation by Mangroves

Otto Richter[1], Hoang Anh Nguyen[1,2] and Van Phuoc Nguyen[2]
[1]Institute of Geoecology, University of Technology Braunschweig, Germany, [2]Institute for Environment & Resources, HCM-City, Vietnam
[1]o.richter@tu-bs.de

Abstract: Metal contaminants and organic pollutants are affecting aquatic environments in urban and industrial zones. Mangrove trees are capable of absorbing metal ions and organic pollutants like PCB and PAH. Located in tidal zones of river estuaries mangrove forests may function as a means for immobilization and removal of pollutants. To estimate the remediation potential of mangroves a two dimensional model of water and substance flow in the soil plant system based on porous media equations is set up based on cohesion-tension theory. In the model, state variables are water potential and contaminant concentrations in the sediment, roots, xylem, core and canopy. Water evaporation from the canopy is taken into account by a transpiration sub model, which is driven by environmental variables such as air water potential, wind speed, radiation and temperature. Boundary conditions at the soil surface are subject to periodical tidal inundations by water with contaminant loads.

Keywords:
Phytoremediation, evapotranspiration, cohesion tension theory, Richards equation

1. Introduction

Mangrove forests deliver many ecosystem services sustaining a large number of human activities comprising fuel collection, fishery and many others [1]. In addition they provide coastal protection and traps for sediments and sinks for nutrients and pollutants. Frequently, mangrove ecosystems in industrial and large urban zones are affected by metal contaminants and organic pollutants. Mangrove trees are capable of absorbing metal ions [2] and organic pollutants like PCB and PAH [3]. Located in tidal zones of river estuaries mangrove forests may function as a means for immobilization and removal of pollutants. It is the purpose of the model presented here to simulate the environmental fate of pollutants in the soil-mangrove system and thus to provide means to quantify its remediation potential. The numerical study is part of a large project comprising experiments for estimating model parameters.

2. Governing equations

A two dimensional model of water and substance flow in the soil plant system based on porous media equations and on plant architecture is set up (Figure 1).

Symbol	meaning
i	index, refers to the compartments soil (s), root (r), xylem (t) and hartwood (k)
ψ_i [cm]	water potential
$\vec{q}_i$ [cm/h]	Darcy velocity
C_i[1/cm]	capacity function
K_i [cm/h]	hydraulic conductivity
$\overline{\overline{D}}_i$	dispersion tensor according to [6]
c_{li}[μ g/l]	liquid phase concentrations
c_{si}[μ g/g]	sorbed phase concentration
θ_i	water content
$K_{d,\,i}$ [ml/g]	partition coefficient
$k_{des,i}$ [1/h]	rate constant for desorption
E	transpiration rate
v	wind velocity
T	temperature
T_x, T_n, T_o	maximum, minimum and optimum temperature
VPD[kPA]	water pressure deficit
PAR	photosynthetic active radiation
$\alpha(\vec{x})$ m^2/m^3	leaf area density at location $\vec{x}$
q_s, q_a	saturation specific humidity
ψ_c	critical leaf water potential
a_i, b_i	parameters of water retention curves in xylem and canopy (eq. 5) according to [5]
g_s [mol/m^2/h]	stomatal conductance
g_{max}	maximal stomatal conductance
a_s	parameter of stomatal conductance
ρ_{air}, ρ_w	density of air and water respectively
$u(z)$	Wind velocity at height z

Table 1. List of symbols

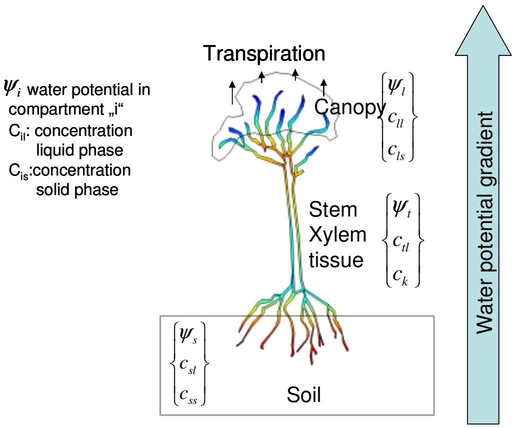

Figure 1. Layout of the model

According to the cohesion-tension theory water transport in the soil and tree is conceived as a continuous hydraulic process, which is driven by canopy transpiration [4]. State variables are water potential and contaminant concentrations in the sediment, roots, xylem, core and canopy. The model equations are obtained by application of Richards equations specific for the soil and each plant compartment. The water transport equations are coupled to the contaminant transport equations via the Darcy velocity and the dispersion tensor. In all compartments, contaminant species can occur in liquid and solid phase. Exchanges between compartments are mediated by a diffusion model on the boundary for transport across membranes. Canopy transpiration is modeled by a sub model, which is driven by environmental variables such as air water potential, wind speed, radiation and temperature. Boundary conditions at the soil surface are subject to periodical tidal inundations by water with contaminant loads. The general form of water and contaminant equations in the root, xylem, core compartments are given by

$$C_i(\psi_i)\frac{\partial \psi_i}{\partial t} = \nabla \cdot K_i(\psi_i)\nabla(\psi_i - z) \quad (1)$$

$$\frac{\partial(\theta_i c_{li})}{\partial t} = \nabla \cdot (\overline{\overline{D}}_i \nabla c_{li} - \vec{q}_i c_{li}) - k_{des,i}(K_{di} c_{li} - c_{si}) \quad (2)$$

$$\frac{\partial}{\partial t} c_{si} = k_{des,i}(K_{di} c_{li} - c_{si}) \quad (3)$$

where the index i refers to the compartments soil (s), root (r), xylem (t) and stem (k) respectively. The second index refers to liquid phase concentrations (l) and solid phase (sorbed) concentrations (s) respectively. In the canopy the following equation holds describing water transport and loss by transpiration

$$C_l(\psi_l)\frac{\partial \psi_l}{\partial t} = \nabla \cdot K_l(\psi_l)\nabla(\psi_l - z) - E(v,T,PAR,VPD,\psi_l,\psi_{air}) \quad (4)$$

In the soil compartment, hydrological conduction and capacity functions are the usual approaches of Van Genuchten and Mualem [5] with parameters appropriate for a sandy soil. The dispersion tensor $\overline{\overline{D}}$ is of the form given by Bear and Buchlin [6]. Retention and capacity functions in the xylem and canopy are taken from [7].

$$\theta_i = a_i - b_i \ln(-\psi_i) \quad (5a)$$

$$C_i = -\frac{b_i}{\psi_i} \quad (5b)$$

where i stands for xylem and canopy respectively. The transpiration sub model is also taken from the publication of Kumagai [7]

$$E(v,T,PAR,VPD,\psi_l,\psi_{air}) = \frac{\rho_{air}}{\rho_w}\alpha(\bar{x})b(z)u(z)(q_s(T_l(z)) - q_a(z)) \quad (6)$$

The bulk transfer coefficient for latent heat b(z) depends on the stomatal conductance g_s, which in turn depends on PAR, temperature, vapor pressure deficit, wind speed at height z and leaf water potential.

$$b(z) = \frac{ch}{1 + ch\frac{\rho_{air}}{g_s}u(z)} \quad (7)$$

The response of stomatal conductance g_s to photosynthetic active radiation PAR, temperature T, vapor pressure deficit VPD and leaf water potential ψ_l is described by the model of Jarvis [8] :

$$g_s = g_{\max} f_P(PAR) f_T(T) f_V(VPD) f_\psi(\psi_l) \qquad (8)$$

where the factors

$$f_P(PAR) = \frac{PAR}{PAR + \dfrac{g_{\max}}{a_s}} \qquad (9)$$

$$f_T(T) = \left(\frac{T - T_n}{T_0 - T_n}\right)\left(\frac{T_x - T}{T_x - T_0}\right)^{(T_x - T_0)/(T_0 - T_n)} \qquad (10)$$

$$f_V(VPD) = \frac{1}{1 + \beta VPD} \qquad (11)$$

and

$$f_\psi(\psi_l) = \frac{1}{1 + \left(\dfrac{\psi_l}{\psi_c}\right)^2} \qquad (12)$$

control stomatal conductance.

3. Use of COMSOL Multiphysics

Boundary conditions at the soil surface are subject to periodical tidal inundations by water with contaminant loads. At the lower boundary a Dirichlet condition with a low water potential near saturation is specified. At the right and left boundaries no flow conditions prevail. Canopy transpiration losses are dependent on time varying environmental conditions, e.g. wind speed and outside air potential. The boundary value problem was implemented into COMSOL using the coefficient form of the PDE interface. Because of the extremely high differences in water potential between air and canopy, boundary and initial conditions and net size and structure had to be set up very carefully in order to achieve convergence.

4. Results

4.1 Constant environmental conditions

The standard run refers to period boundary conditions due to the diurnal variation of PAR, all other environmental variables held constant. Figure 2.1 shows a snapshot of the water potential at time t = 4 h. Figure 2.2 shows a snapshot of the distribution of pollutant concentrations at time t = 4 h. Water uptake by the roots causes a sharp decrease of the water potential in the root zone (cf. also Figure 2.3).

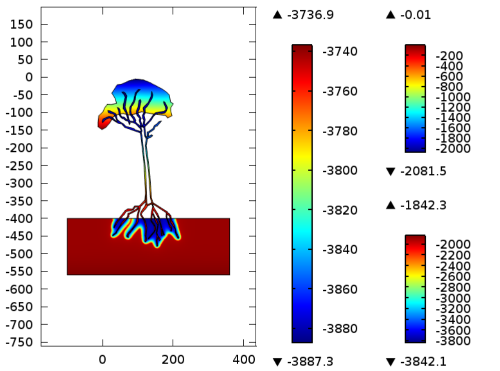

Figure 2.1 Water potential in cm. Note that the color legend is specific for each compartment. Left: leaf, right, top: xylem, right, bottom: soil

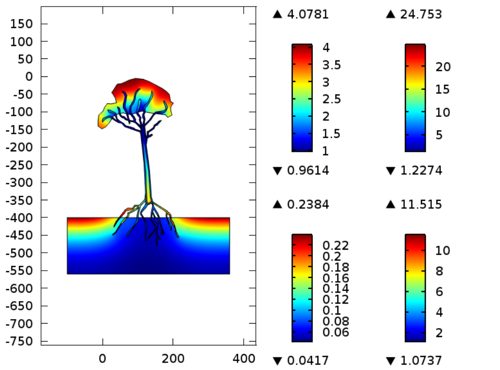

Figure 2.2. Pollutant concentrations in g/kg. Note that the color legend is specific for each compartment. Left, top: core, right, top: soil, left, bottom: leaves, right bottom: xylem.

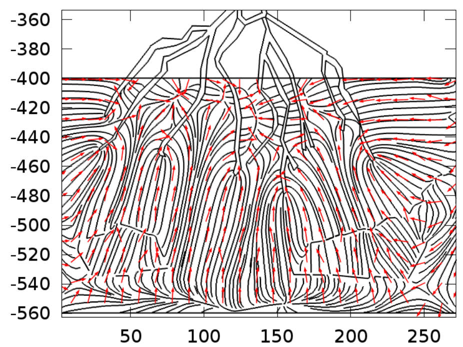

Figure 2.3. Streamlines in the root zone at t = 14.5 h.

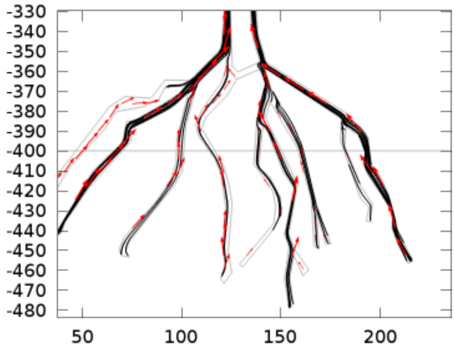

Figure 2.4. Streamlines in xylem at t = 14.5 h.

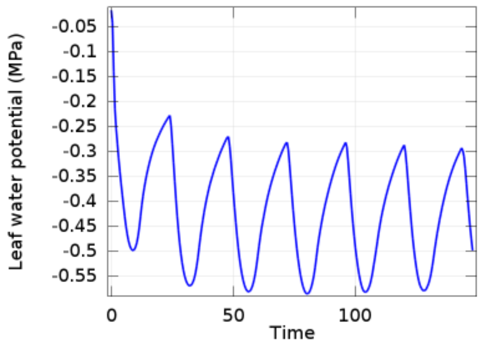

Figure 2.5. Point graph of diurnal variation of leaf water potential at some point in the canopy.

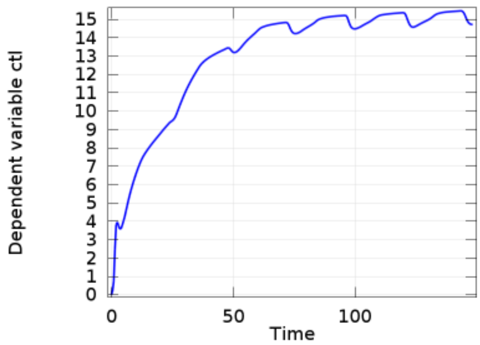

Figure 2.6. Point graph of diurnal variation of pollutant concentration in roots.

Figures 2.3 and 2.4 show snapshots of the streamlines in soil and xylem respectively. The diurnal variation of the photosynthetic active radiation causes a period change of transpiration as can be seen from equation 9. This variation is shown in the time course of leaf water potential (Figure 2.5) and also in the time course of concentrations in the compartments as shown in figure 2.6 for a point in the roots.

4.2 Wind and tidal inundations

Transpiration is driven by wind (cf. equation 6). In the following simulation the model response to variations in wind velocity was studied.

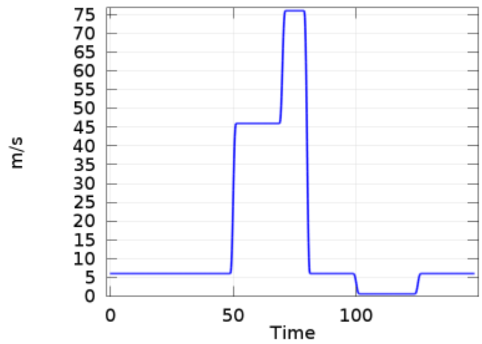

Figure 3.1. Variation of above canopy wind speed.

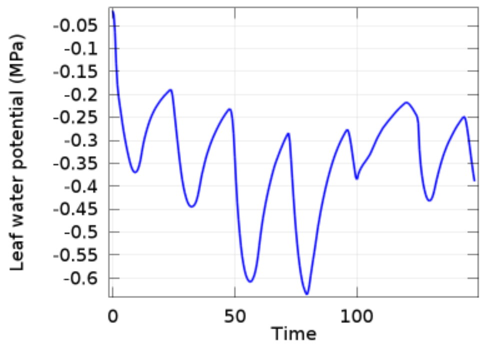

Figure 3.2. Point graph of diurnal variation of leaf water potential under the time course of the wind speed shown in preceding figure.

Typically mangroves grow in the tidal zone and are subject to periodic tidal inundations. This was modeled by a periodic change of the upper flow boundary condition of the soil compartment. Figure 3.3 shows the time course of concentrations at a point near the boundary. Note that both the diurnal variation of the photosynthetic active radiation via the evaporation and the inundation influence the infiltration resulting in a irregular curve. This is also seen in the time course at point in the roots as shown in Figure 3.4.

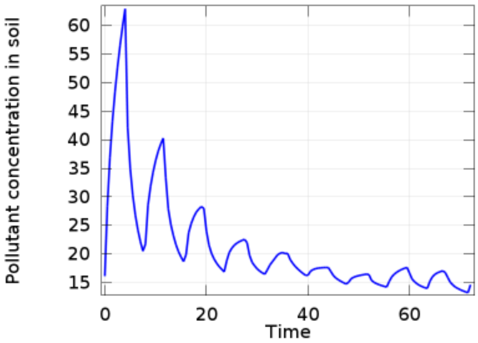

Figure 3.3. Point graph of variation of pollutant concentration in soil (near upper boundary) under the combined influence of tide and diurnal variation of leaf water potential.

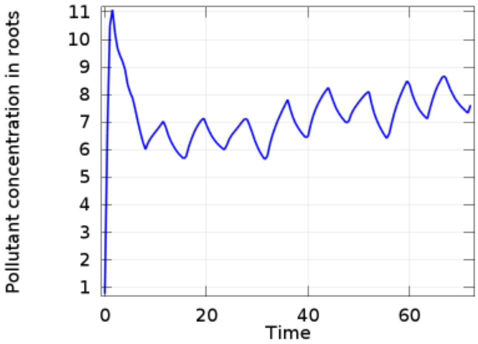

Figure 3.4. Point graph of variation of pollutant concentration in the roots under the combined influence of tide and diurnal variation of leaf water potential (cf. figure 2.5).

5. Summary and conclusions

We have shown that multiphysics approaches also apply to biological systems. Here, we have coupled hydrological processes with biological processes by use of partial differential equations based on transport theory for porous media. Evaporation is controlled by stomatal opening and closing, which in turn is governed by intrinsic biological regulation mechanisms. The model is capable of simulating water flow from roots to canopy and the uptake and transport of chemicals. The model responses to changing environmental conditions -wind speed and inundations- in a reasonable way. In order to use the model for the estimation of the phytoremediation potential, parameters specific for pollutants such as metals or organic compounds have to be identified. To this end experiments with designs guided by the need of parameter estimation are being set up where young mangrove plants are exposed to pollutants of different loads, which will then be measured in the organs of the plants.

6. References

1. Lucy, E, Counting mangrove ecosystems as economic components of Asia's coastal infrastructure, *Proceedings of International Conference and Exhibition on Mangroves of Indian and Western Pacific Oceans*, (Iceman 2006), Aug 21-24, Kuala Lumpur, pp. 1-14

2. V Pahalawattarachchi, C S Purushothaman & A Vennila, Metal phytoremediation potential of Rhizophora mucronata (Lam.), *Indian Journal of Marine Sciences* **Vol. 38** (2, pp. 178-183 (2009)

3. Bo Zhao, Yan-wu Zhou & Gui-zhu Chen, The effect of mangrove reforestation on the accumulation of PCBs in sediment from different habitats in Guangdong, China, *Marine Pollution Bulletin* **64**, pp 1614-1619, 2012

4. Janott, M., Gayler, S., Gessler, A., Javaux, M., Klier, C. and Priesack, M., A one-dimensional model of water flow in soil-plant systems based on plant architecture, *Plant Soil* **341**:233-256 (2011)

5. van Genuchten, M. Th. (1980), A closed-form equation for predicting the hydraulic conductivity of unsaturated soils, *Madison. Soil Sci. Soc. Am. J.* **44**: 892-898

6. Bear J. and Buchlin J. M. *in"Modelling and Application of Transport Phenomena in Porous Media"*, pp 154-157, Kluver Academic Publishers, Dordrecht 1991

7. Kumagai, T., Modeling water transportation and storage in sapwood - model development and validation, *Agricultural and Forest meteorology* **109**, pp 105-115 (2001)

8. Jarvis, P.G., The interpretation of the variations in leaf water potential and stomatal conductance found in canopies in the field. *Philos.Trans.R.Soc.*, London, Ser. **B** **273**,593-610 (1976)